

=> d his

(FILE 'HOME' ENTERED AT 11:19:30 ON 06 MAY 2001)

FILE 'REGISTRY' ENTERED AT 11:19:42 ON 06 MAY 2001

L1 STRUCTURE UPLOADED  
L2 50 S L1  
L3 STRUCTURE UPLOADED  
L4 50 S L3  
L5 STRUCTURE UPLOADED  
L6 35 S L5  
L7 428 S L5 FULL

FILE 'CAPLUS, USPATFULL' ENTERED AT 11:23:09 ON 06 MAY 2001

L8 452 S L7  
L9 10 S L8 AND ((CA OR CALCIUM) (P) CHANNEL)  
L10 10 DUP REM L9 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 11:28:55 ON 06 MAY 2001

L11 2 S MIBEFRADIL  
L12 87 S L8 AND ?BIS

FILE 'CAPLUS, USPATFULL' ENTERED AT 11:36:48 ON 06 MAY 2001

L13 98 S L8 AND BIS?  
L14 4 S L8 AND DIMER

FILE 'STNGUIDE' ENTERED AT 11:41:50 ON 06 MAY 2001

FILE 'REGISTRY' ENTERED AT 11:45:18 ON 06 MAY 2001

L15 STRUCTURE UPLOADED  
L16 3 S L15  
L17 31 S L15 FULL

FILE 'CAPLUS, USPATFULL, MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001

L18 11 S L17

FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001

L19 3 S CLENTIAZEM

FILE 'CAPLUS' ENTERED AT 11:48:39 ON 06 MAY 2001

FILE 'REGISTRY' ENTERED AT 11:48:42 ON 06 MAY 2001

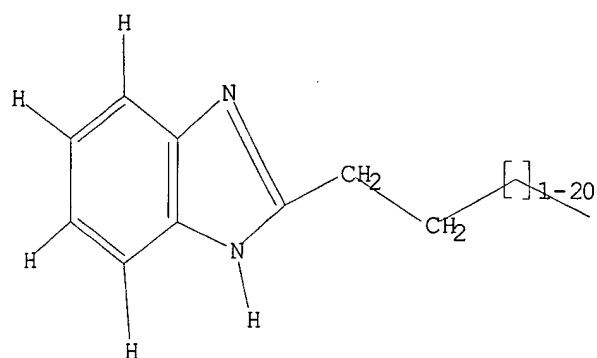
FILE 'REGISTRY' ENTERED AT 11:49:12 ON 06 MAY 2001

L20 21 S DILTIAZEM

=> d 15

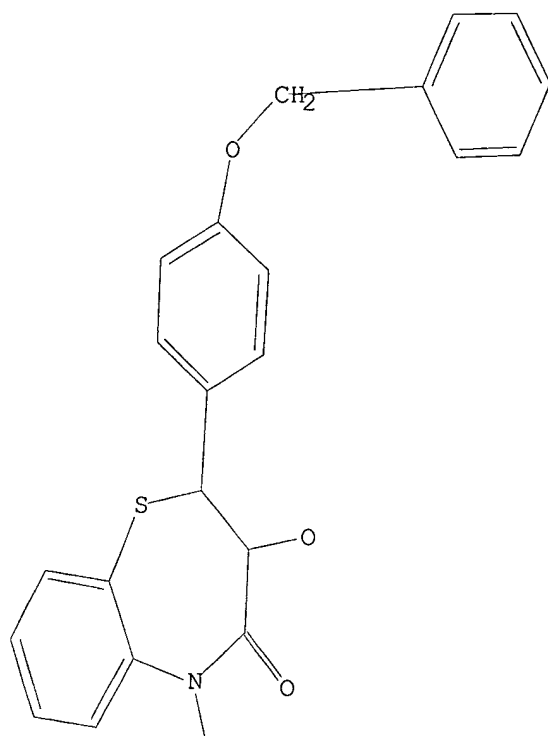
L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> d 115  
 L15 HAS NO ANSWERS  
 L15 STR



Structure attributes must be viewed using STN Express query preparation.

=>

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:776400 CAPLUS

DOCUMENT NUMBER: 123:245168

TITLE: Synthesis, Characterization, Spectroscopy, and Magnetism of Dinuclear Azido- and Alkoxo-Bridged Copper(II) Complexes of Bis(2-benzimidazolyl)alkanes. X-ray Structures of

[Cu<sub>2</sub>(tbz)<sub>2</sub>(CH<sub>3</sub>O)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>(CH<sub>3</sub>OH)<sub>2</sub>,

[Cu<sub>2</sub>(tbz)<sub>2</sub>(NO<sub>3</sub>)(CH<sub>3</sub>O)<sub>2</sub>](NO<sub>3</sub>)(CH<sub>3</sub>OH)<sub>2</sub>, and

[Cu(tbz)(N<sub>3</sub>)<sub>2</sub>]<sub>2</sub>(CH<sub>3</sub>OH)<sub>2</sub> (tbz = Bis(2-benzimidazolyl)propane)

AUTHOR(S): Van Albada, Gerard A.; Lakin, Miles T.; Veldman, Nora;

Spek, Anthony L.; Reedijk, Jan

CORPORATE SOURCE: Leiden Institute of Chemistry, Leiden University, Leiden, 2300 RA, Neth.

SOURCE: Inorg. Chem. (1995), 34(19), 4910-17

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A group of new compds. Cu(L)(sol-)(A-)(Hsol), where A = ClO<sub>4</sub>-, CF<sub>3</sub>SO<sub>3</sub>-, BF<sub>4</sub>-, and NO<sub>3</sub>-, L = bis(2-benzimidazolyl)propane (abbreviated as tbz) and bis(2-benzimidazolyl)butane (abbreviated as qbz), and Hsol = MeOH and EtOH, and [Cu(tbz)(N<sub>3</sub>)(Hsol)] was prepd. and characterized structurally, magnetically, and spectroscopically. Three representative compds. [Cu<sub>2</sub>(tbz)<sub>2</sub>(MeO)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>(MeOH)<sub>2</sub> (1), [Cu<sub>2</sub>(tbz)<sub>2</sub>(NO<sub>3</sub>)(MeO)<sub>2</sub>](NO<sub>3</sub>)(MeOH)<sub>2</sub> (5), and [Cu(tbz)(N<sub>3</sub>)<sub>2</sub>]<sub>2</sub>(MeOH)<sub>2</sub> (13) were characterized structurally with x-ray diffraction. Crystal data for 1: monoclinic, space group P2<sub>1</sub>/c

with

a 9.6863(10), b 12.9445(10), c 19.394(2) .ANG., .beta.

113.259(10).degree., and Z = 2. Crystal data for 5: monoclinic, space group P2<sub>1</sub> with a 9.5497(6), b 12.5073(7), c 17.5920(12) .ANG., .beta.

90.996(6).degree., and Z = 2. Crystal data for 13: orthorhombic, space group Pbc<sub>a</sub> with a 11.3325(7), b 18.7096(16), c 19.2011(16) .ANG., and Z =

4. The structure refinement converged to wR<sub>2</sub> = 0.1381, R<sub>1</sub> = 0.0534 for

1,

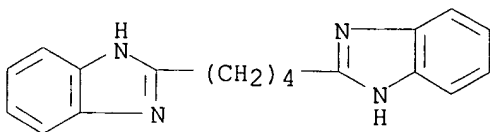
wR<sub>2</sub> = 0.0674, R<sub>1</sub> = 0.0271 for 5, and wR<sub>2</sub> = 0.1119, R<sub>1</sub> = 0.0701 for 13.

The structures 1 and 5 consist of dinuclear units with bridging methoxo groups and one ligand linked to each Cu via the N, providing square

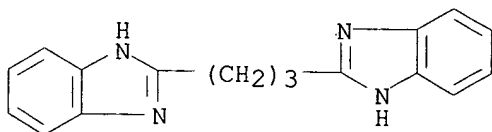
planar

CuN<sub>2</sub>O<sub>2</sub> chromophores. Structure 5 consists of a dinuclear unit in which one of the Cu atoms is linked to a nitrate O, to yield a unit with two different Cu environments, one square planar and the other square pyramidal. Structure 13 consists also of dinuclear units with the two Cu atoms bridged by .mu.-(1,1)-azido groups. Also each Cu is surrounded by two nitrogens of the ligand and a N of a nonbridging end-on .mu.-(1,1)-azido moiety resulting in a distorted square pyramidal geometry. The Cu-Cu distances (.ANG.) within the dinuclear units are as follows: 1, 2.9827(6); 5, 3.0072(4); 13, 3.2422(9). The Cu-O-Cu bridging angles (deg) are as follows: 1, 102.89(14); 5, 103.97(9), 103.06(9).degree.. The Cu-N-Cu bridging angle for 13 is 104.66(17).degree.. Far-IR spectroscopy shows bands which are characteristic for the bridging Cu<sub>2</sub>O<sub>2</sub>N<sub>4</sub> chromophore; Cu-O vibrations are found at .apprx.457 and 330 cm<sup>-1</sup> for the ethoxo-bridged compds. and at .apprx.390 and 232 cm<sup>-1</sup> for the methoxo-bridged compds. The magnetic susceptibility measurements of the alkoxo-bridged compds. display a diamagnetic behavior below room temp. with an estd. exchange parameter 2J of <-600 cm<sup>-1</sup>. These dinuclear species are EPR silent, and only a weak signal of monomeric impurities is obsd. The .mu.-(1,1)-azido-bridged dimer shows a ferromagnetic behavior with a calcd. J value of +23

cm-1 and a weak, very broad isotropic EPR signal at  $g = 2.14$ .  
 IT 4746-56-9, 1,4-Bis(2-benzimidazolyl)butane  
 RL: RCT (Reactant)  
 (for prepn. of copper dinuclear alkoxo-bridged complexes)  
 RN 4746-56-9 CAPLUS  
 CN 1H-Benzimidazole, 2,2'-(1,4-butanediyl)bis- (9CI) (CA INDEX NAME)



IT 7147-66-2, 1,3-Bis(2-benzimidazolyl)propane  
 RL: RCT (Reactant)  
 (for prepn. of copper dinuclear azido-, alkoxo- and  
 alkoxo/nitrato-bridged complexes)  
 RN 7147-66-2 CAPLUS  
 CN 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis- (9CI) (CA INDEX NAME)



=>

=> s l15 full  
FULL SEARCH INITIATED 11:46:09 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 389 TO ITERATE

100.0% PROCESSED 389 ITERATIONS  
SEARCH TIME: 00.00.01

L17 31 SEA SSS FUL L15

=> file caplu uspatful medlin  
COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE TOTAL  
ENTRY SESSION  
133.87 368.41

SINCE FILE TOTAL  
ENTRY SESSION  
0.00 -1.18

FILE 'CAPLUS' ENTERED AT 11:46:19 ON 06 MAY 2001  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE 'USPATFULL' ENTERED AT 11:46:19 ON 06 MAY 2001  
CA INDEXING COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001

=> s l17  
L18 11 L17

=> d hitstr 1-  
YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L18 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2001 ACS

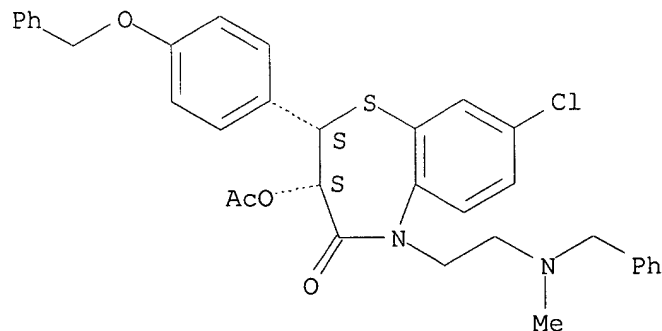
IT 112525-50-5P 112525-51-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for clentiazem metabolite)

RN 112525-50-5 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-  
[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

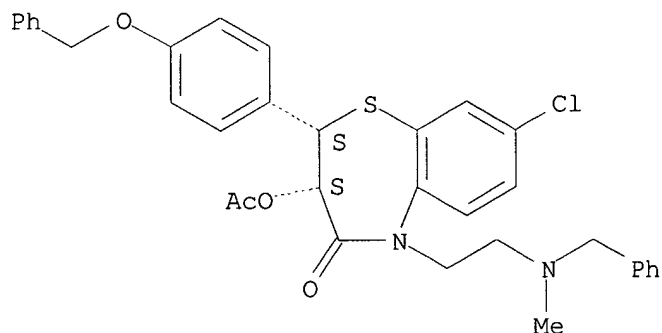


RN 112525-51-6 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

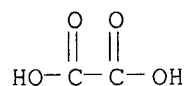
CRN 112525-50-5  
 CMF C34 H33 Cl N2 O4 S  
 CDES \*

Absolute stereochemistry.



CM 2

CRN 144-62-7  
 CMF C2 H2 O4



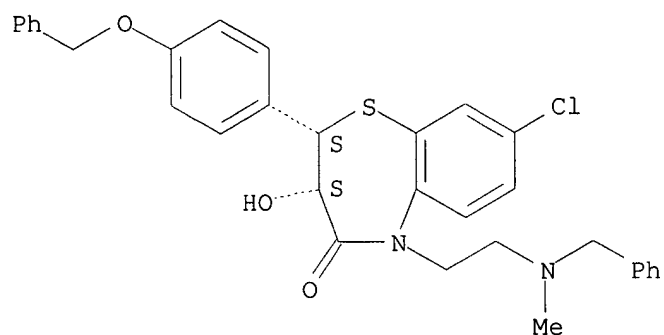
IT 112525-30-1P 112525-31-2P 112525-45-8P  
 112525-46-9P 112525-54-9P 112544-49-7P  
 156415-90-6P 156415-91-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, clentiazem metabolite)

RN 112525-30-1 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-2,3-dihydro-3-hydroxy-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

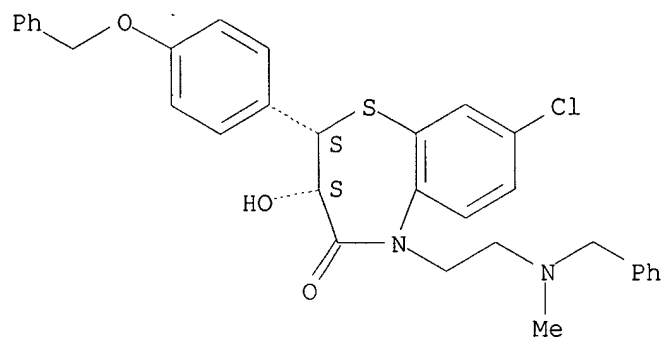


RN 112525-31-2 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-2,3-dihydro-3-hydroxy-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

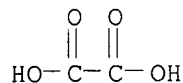
CRN 112525-30-1  
 CMF C32 H31 Cl N2 O3 S  
 CDES \*

Absolute stereochemistry.



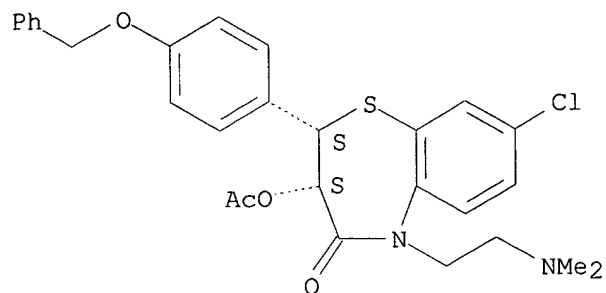
CM 2

CRN 144-62-7  
 CMF C2 H2 O4



RN 112525-45-8 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

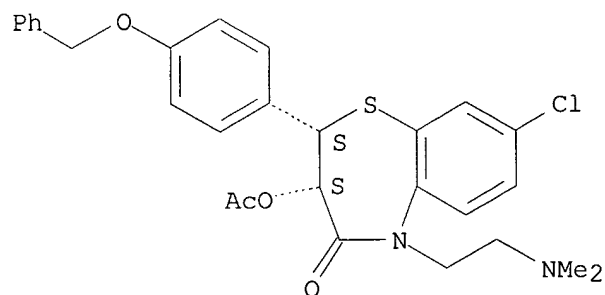


RN 112525-46-9 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

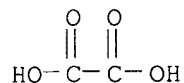
CRN 112525-45-8  
 CMF C28 H29 Cl N2 O4 S  
 CDES \*

Absolute stereochemistry.



CM 2

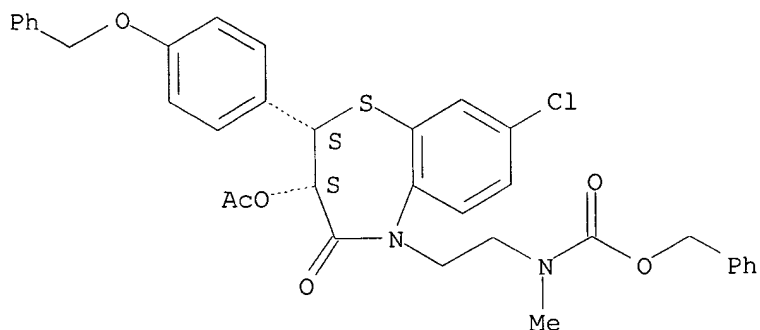
CRN 144-62-7  
 CMF C2 H2 O4



RN 112525-54-9 CAPLUS  
 CN Carbamic acid, [2-[3-(acetyloxy)-8-chloro-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

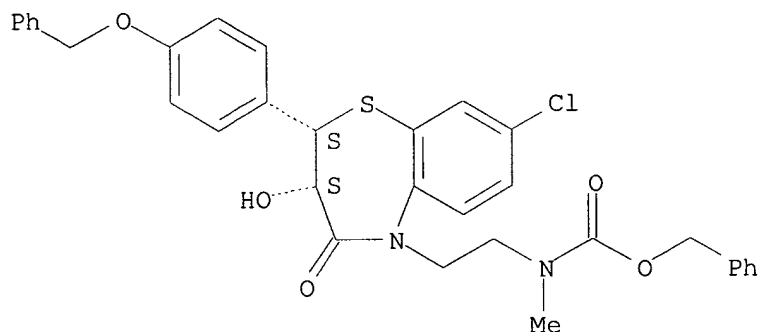




RN 112544-49-7 CAPLUS

CN Carbamic acid, [2-[8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

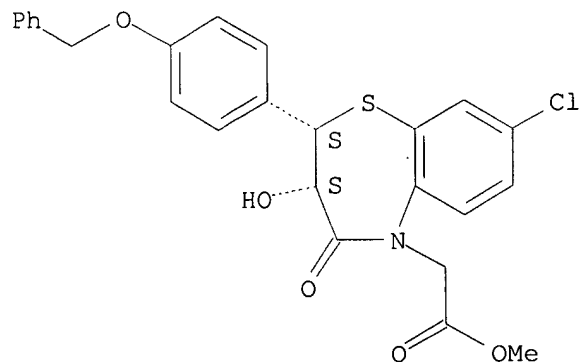


RN 156415-90-6 CAPLUS

CN 1,5-Benzothiazepine-5(2H)-acetic acid, 8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-, methyl ester, (2S-cis)- (9CI) (CA

INDEX  
NAME)

Absolute stereochemistry.

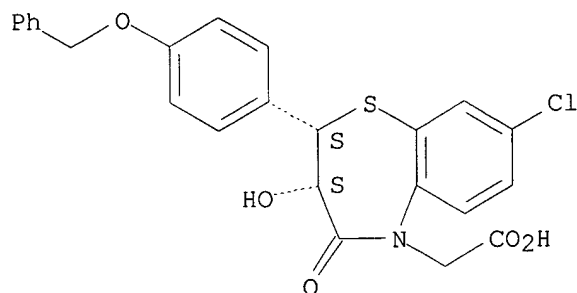


RN 156415-91-7 CAPLUS

CN 1,5-Benzothiazepine-5(2H)-acetic acid, 8-chloro-3,4-dihydro-3-hydroxy-4-

oxo-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2001 ACS

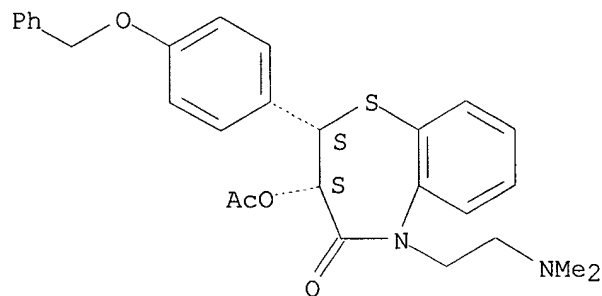
IT 84903-76-4P 142843-03-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and deprotection of)

RN 84903-76-4 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one,  
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

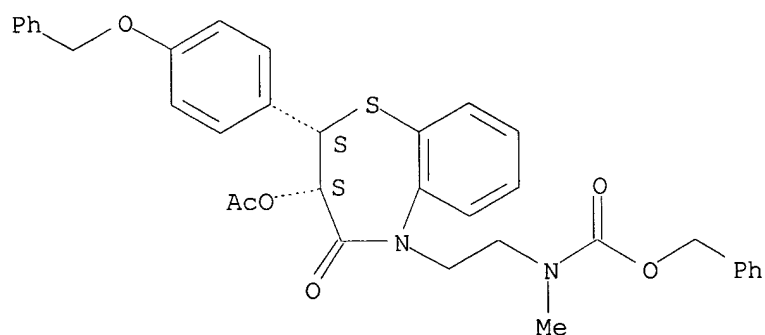
Relative stereochemistry.



RN 142843-03-6 CAPLUS

CN Carbamic acid, [2-[3-(acetyloxy)-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 142843-01-4P 142843-02-5P

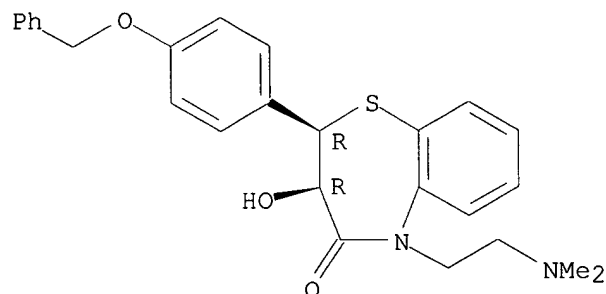
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn., acetylation, and deprotection of)

RN 142843-01-4 CAPLUS

RN 142843-02-5 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2001 ACS

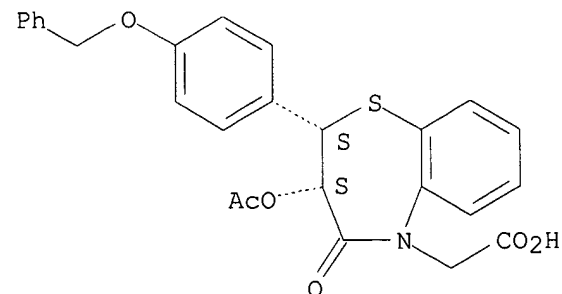
IT 115973-34-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and debenzylation of)

RN 115973-34-7 CAPLUS

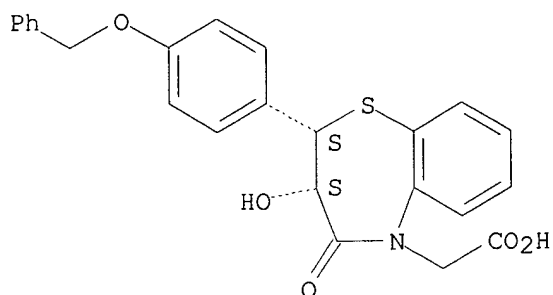
CN 1,5-Benzothiazepine-5(2H)-acetic acid, 3-(acetyloxy)-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



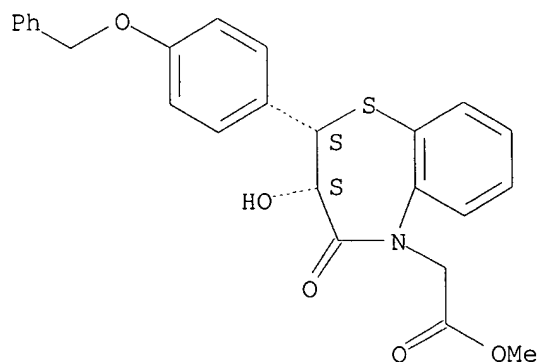
IT **115973-33-6P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and debenzoylation or acetylation of)  
 RN 115973-33-6 CAPLUS  
 CN 1,5-Benzothiazepine-5(2H)-acetic acid, 3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **115992-92-2P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and hydrolysis of)  
 RN 115992-92-2 CAPLUS  
 CN 1,5-Benzothiazepine-5(2H)-acetic acid, 3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-, methyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2001 ACS

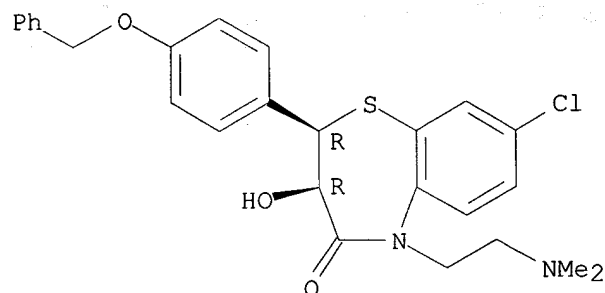
IT **112525-38-9P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and acetylation of)  
 RN 112525-38-9 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 112525-37-8  
 CMF C26 H27 Cl N2 O3 S

CDES 2:CIS3:(+)

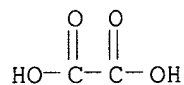
Rotation (+). Absolute stereochemistry unknown.



CM 2

CRN 144-62-7

CMF C2 H2 O4



IT 112525-31-2P 112525-51-6P 112525-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and debenzoylation and N-acylation of)

RN 112525-31-2 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-2,3-dihydro-3-hydroxy-5-[2-  
[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-,  
(2S-cis)-,

ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

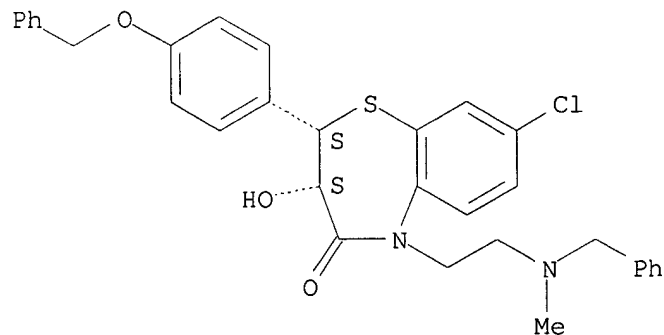
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CRN 112525-30-1

CMF C32 H31 Cl N2 O3 S

CDES \*

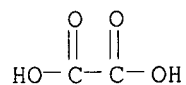
Absolute stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 112525-51-6 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

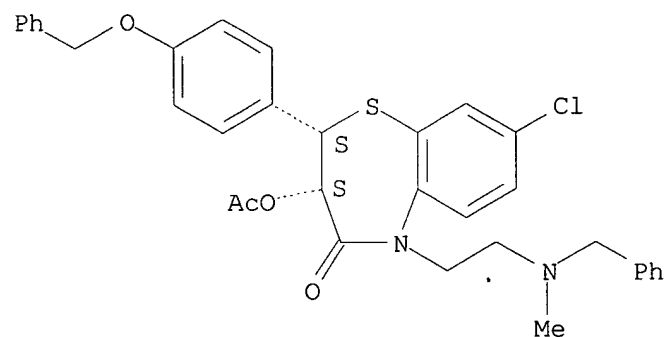
CM 1

CRN 112525-50-5

CMF C34 H33 Cl N2 O4 S

CDES \*

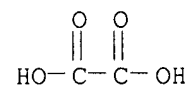
Absolute stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



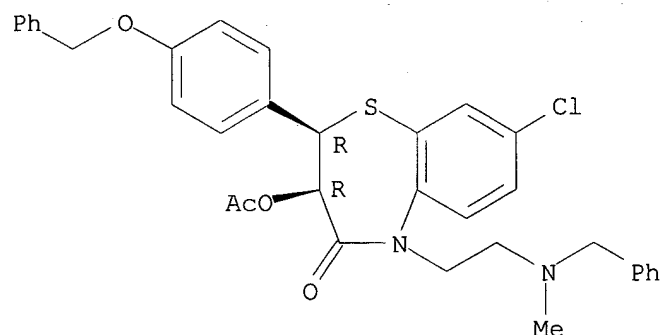
RN 112525-53-8 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-2,3-dihydro-5-[2-[methyl(phenylmethyl)amino]ethyl]-2-[4-(phenylmethoxy)phenyl]-, (2R-cis)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

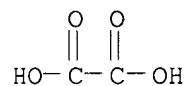
CRN 112525-52-7  
 CMF C34 H33 Cl N2 O4 S  
 CDES \*

Absolute stereochemistry.



CM 2

CRN 144-62-7  
 CMF C2 H2 O4



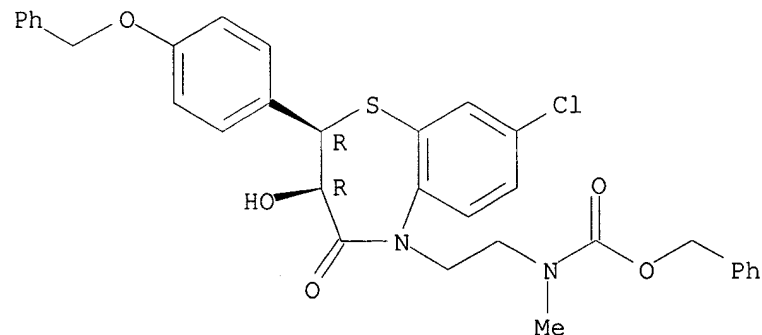
IT 112525-34-5P 112525-46-9P 112525-54-9P  
 112544-49-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and deprotection of)

RN 112525-34-5 CAPLUS

CN Carbamic acid, [2-[8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 112525-46-9 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, (2S-cis)-,

ethanedioate (2:1) (9CI) (CA INDEX NAME)

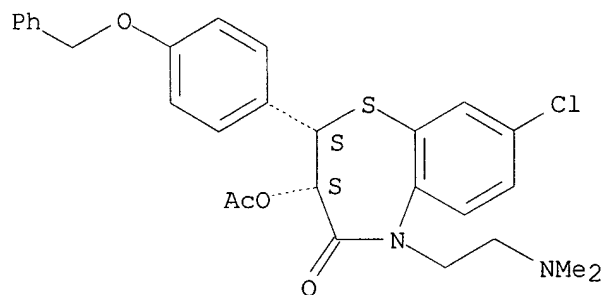
CM 1

CRN 112525-45-8

CMF C28 H29 Cl N2 O4 S

CDES \*

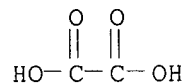
Absolute stereochemistry.



CM 2

CRN 144-62-7

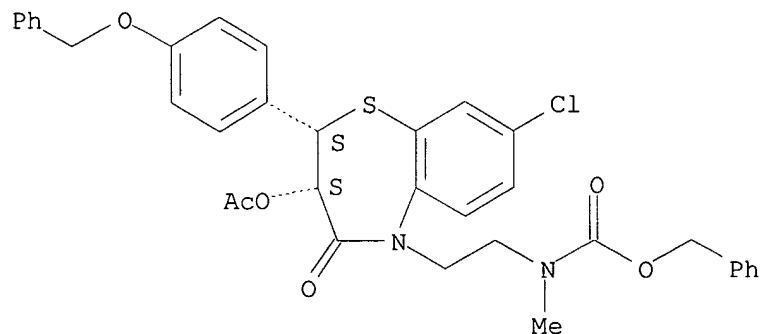
CMF C2 H2 O4



RN 112525-54-9 CAPLUS

CN Carbamic acid, [2-[3-(acetyloxy)-8-chloro-3,4-dihydro-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

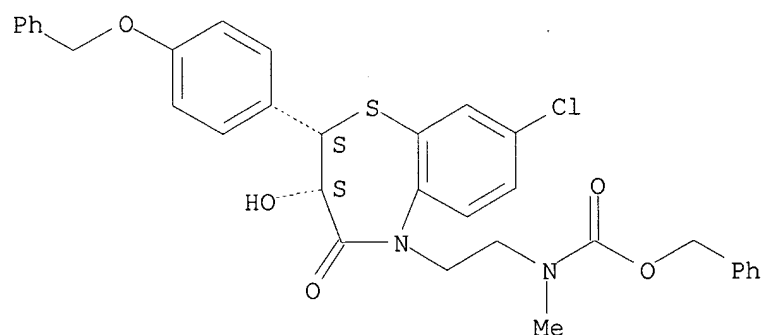


RN 112544-49-7 CAPLUS

CN Carbamic acid, [2-[8-chloro-3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, (2S-cis)- (9CI) (CA INDEX NAME)



Absolute stereochemistry.



IT 112525-40-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for cardiovascular agent)

RN 112525-40-3 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(-)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

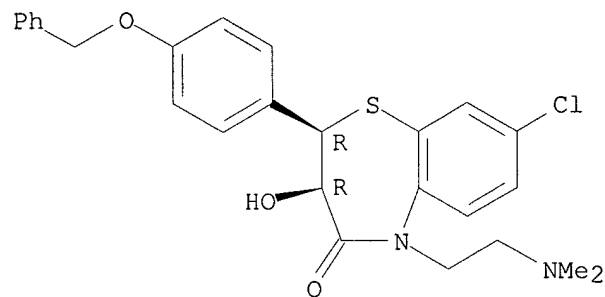
CM 1

CRN 112525-39-0

CMF C26 H27 Cl N2 O3 S

CDES 2:CIS3: (-)

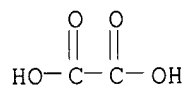
Rotation (-). Absolute stereochemistry unknown.



CM 2

CRN 144-62-7

CMF C2 H2 O4



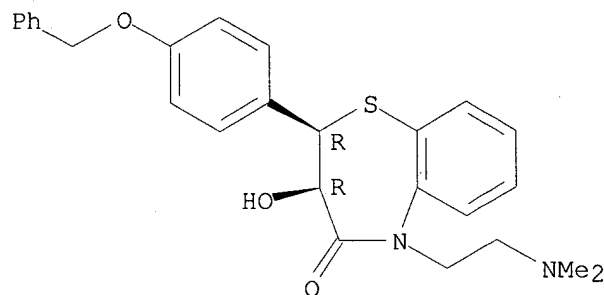
IT 84903-70-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and acetylation of)

RN 84903-70-8 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



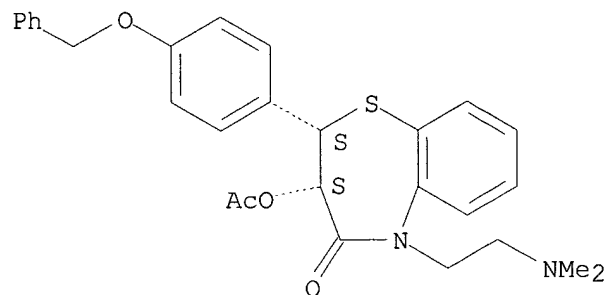
IT 84903-71-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 84903-71-9 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



L18 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2001 ACS

IT 84903-70-8P 84903-71-9P 84903-72-0P

84903-73-1P 84903-74-2P 84903-75-3P

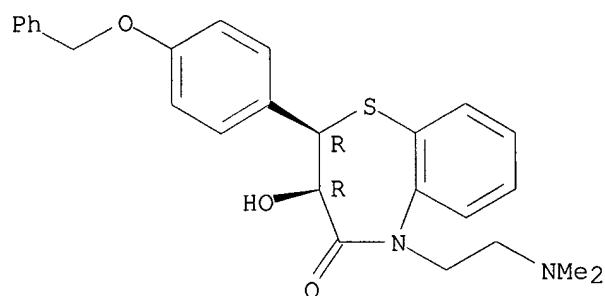
84903-76-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 84903-70-8 CAPLUS

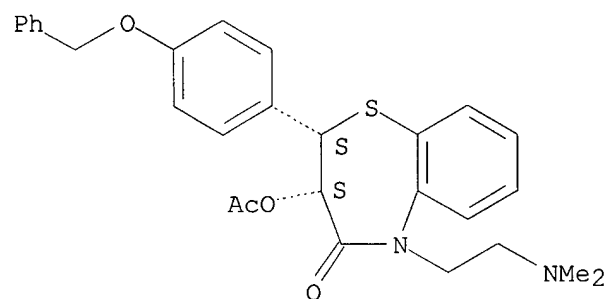
CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



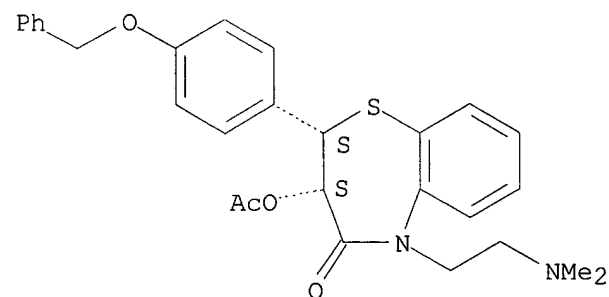
RN 84903-71-9 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 84903-72-0 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, cis-(+)- (9CI)  
 (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

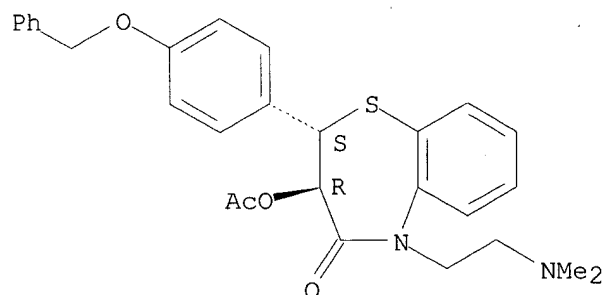


HCl

RN 84903-73-1 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-

dihydro-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 84903-74-2 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one,

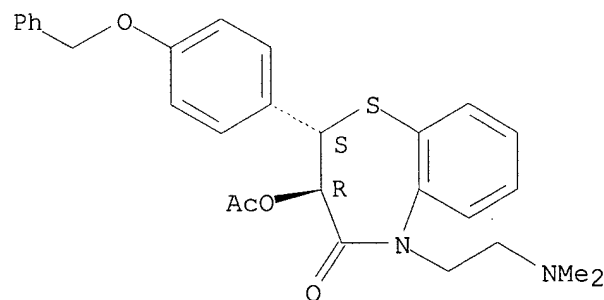
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-

dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, trans- (9CI)

(CA

INDEX NAME)

Relative stereochemistry.



● HCl

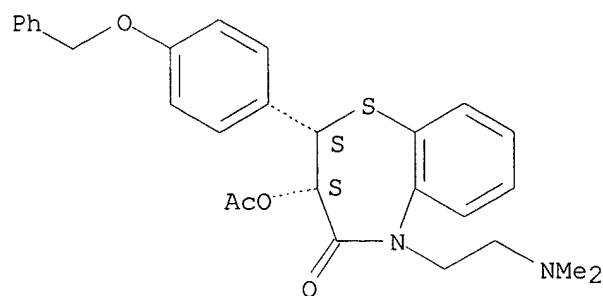
RN 84903-75-3 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one,

3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-

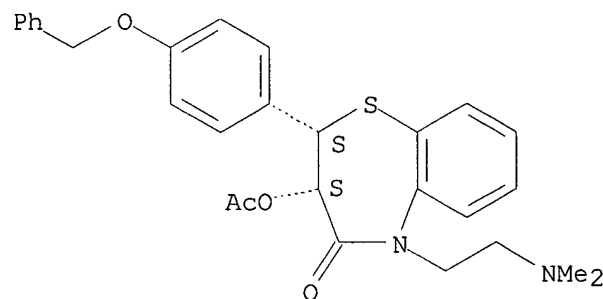
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



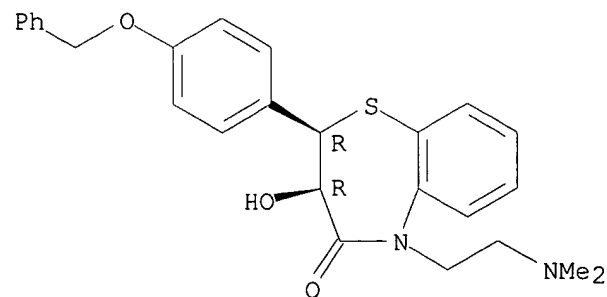
RN 84903-76-4 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 IT **84903-70-8P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and acetylation of)  
 RN 84903-70-8 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-  
 hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

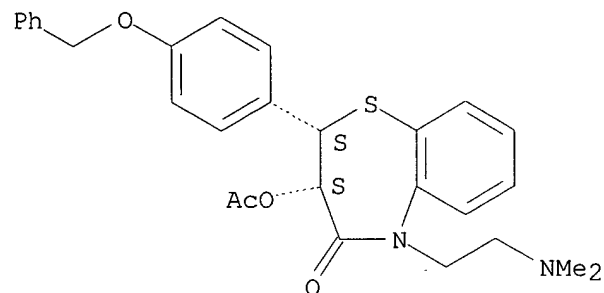
Rotation (+). Absolute stereochemistry unknown.



IT **84903-71-9P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and debenzoylation of)

RN 84903-71-9 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



L18 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2001 ACS

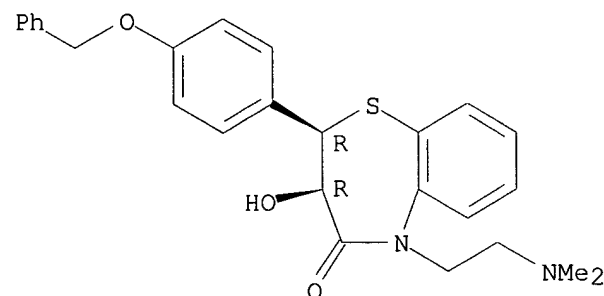
IT **84903-70-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and acetylation of)

RN 84903-70-8 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-  
 hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



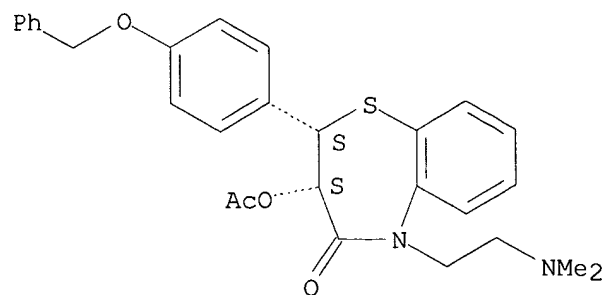
IT **84903-71-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and debenzoylation of)

RN 84903-71-9 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



L18 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2001 ACS

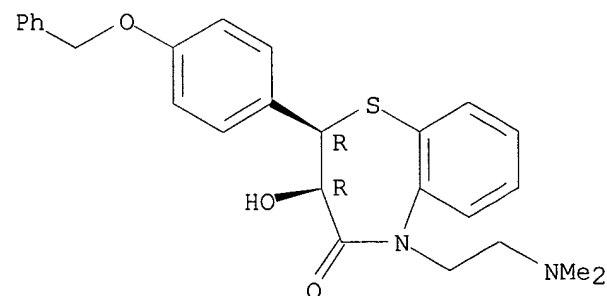
IT **84903-70-8P 84914-79-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and acetylation of)

RN 84903-70-8 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

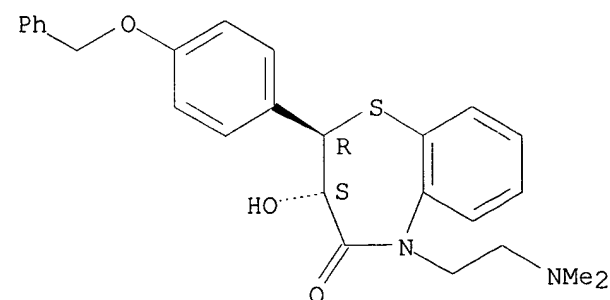
Rotation (+). Absolute stereochemistry unknown.



RN 84914-79-4 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



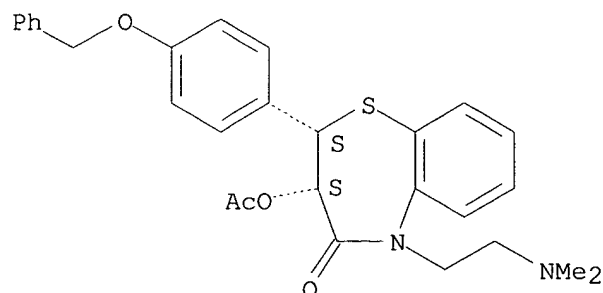
IT **84903-71-9P 84903-73-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and debenzoylation of)

RN 84903-71-9 CAPLUS

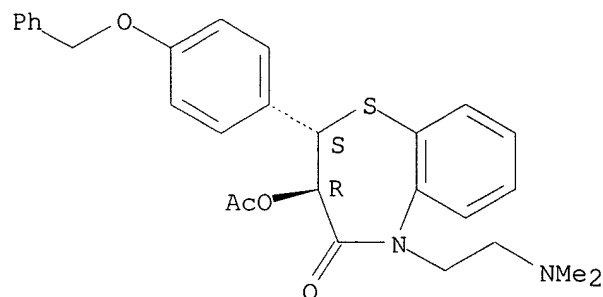
CN 1,5-Benzothiazepin-4(5H)-one,  
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 84903-73-1 CAPLUS  
CN 1,5-Benzothiazepin-4(5H)-one,  
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
dihydro-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2001 ACS

IT **84903-70-8P**

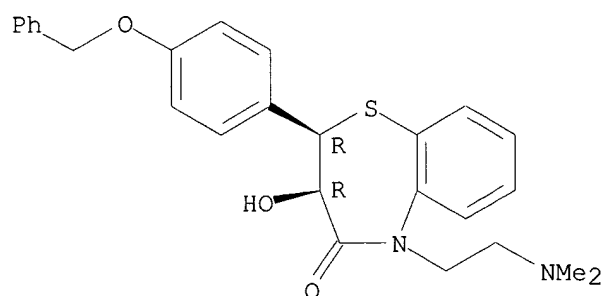
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and acetylation of)

RN 84903-70-8 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-  
hydroxy-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.





IT 84903-71-9P 84903-72-0P 84903-73-1P

84903-74-2P 84903-75-3P 84903-76-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

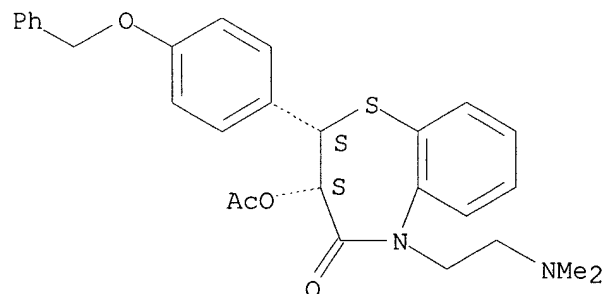
RN 84903-71-9 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one,

3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-

dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



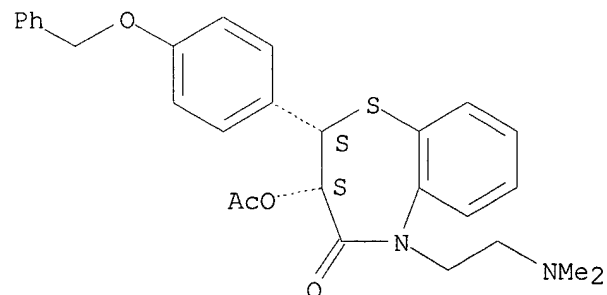
RN 84903-72-0 CAPLUS

CN 1,5-Benzothiazepin-4(5H)-one,

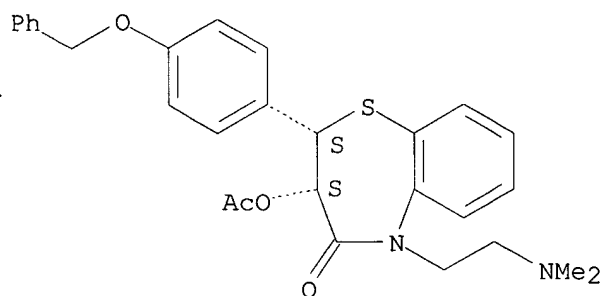
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-

dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, cis-(+)- (9CI)  
(CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



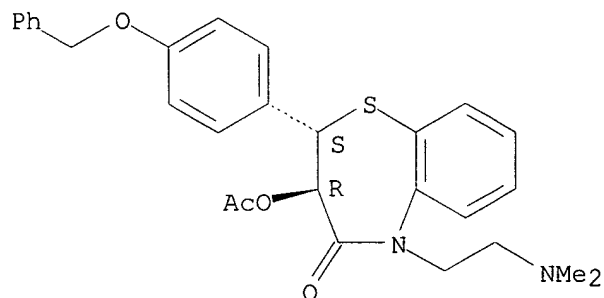
● HCl



● HCl

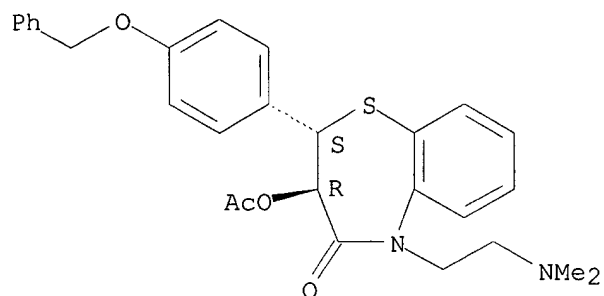
RN 84903-73-1 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 84903-74-2 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, monohydrochloride, trans- (9CI)  
 (CA  
 INDEX NAME)

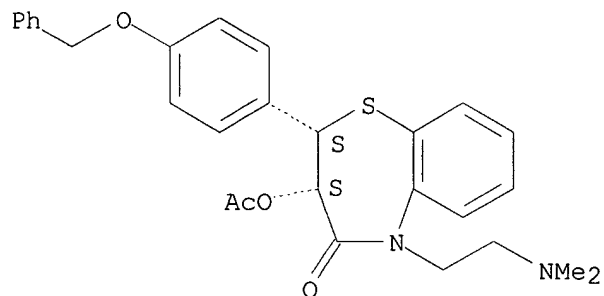
Relative stereochemistry.



● HCl

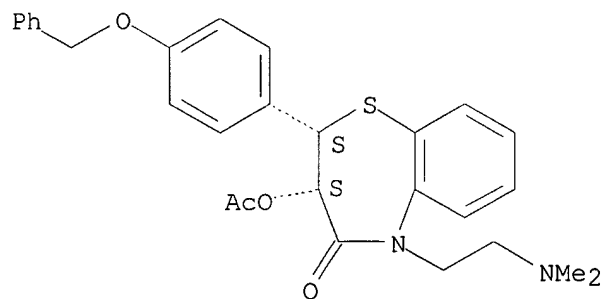
RN 84903-75-3 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, cis-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



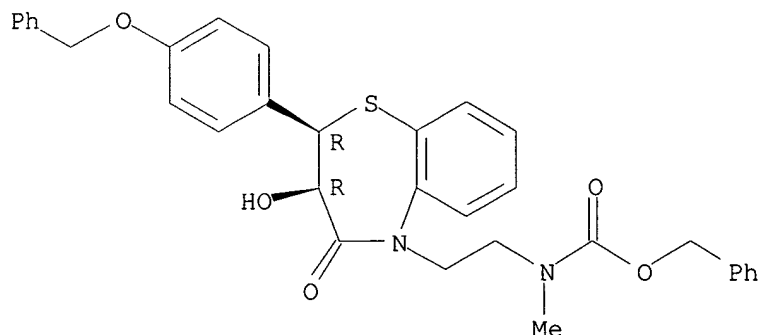
RN 84903-76-4 CAPLUS  
 CN 1,5-Benzothiazepin-4(5H)-one,  
 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-  
 dihydro-2-[4-(phenylmethoxy)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and hydrolysis of)  
 RN 68767-01-1 CAPLUS  
 CN Carbamic acid,  
 [2-[3,4-dihydro-3-hydroxy-4-oxo-2-[4-(phenylmethoxy)phenyl]-  
 1,5-benzothiazepin-5(2H)-yl]ethyl]methyl-, phenylmethyl ester, cis- (9CI)  
 (CA INDEX NAME)

Relative stereochemistry.



=> d ti

L18 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI Synthesis of the metabolites of clentiazem

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	25.74	394.15
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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STRUCTURE FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3  
 DICTIONARY FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
 for details.

=> s clentiazem

L19 3 CLENTIAZEM

=> d

L19 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2001 ACS

RN 96128-92-6 REGISTRY

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S,3S)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-8-chloro-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S-cis)-, (Z)-2-butenedioate (1:1)

OTHER NAMES:

CN (S,S)-Clentiazem maleate

CN Clentiazem maleate

CN TA 3090

FS STEREOSEARCH

MF C22 H25 Cl N2 O4 S . C4 H4 O4

CI COM

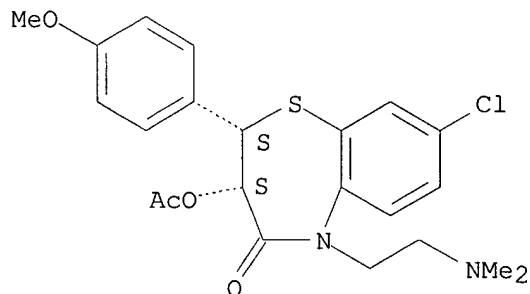
LC STN Files: BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, DDFU, DRUGPAT, DRUGU, DRUGUPDATES, EMBASE, IPA, MRCK\*, PHAR, PROMT, RTECS\*, SYNTHLINE, TOXLINE, TOXLIT, USAN, USPATFULL  
(\*File contains numerically searchable property data)

CM 1

CRN 96125-53-0

CMF C22 H25 Cl N2 O4 S

Absolute stereochemistry.

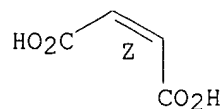


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



48 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

48 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 11:19:30 ON 06 MAY 2001)

FILE 'REGISTRY' ENTERED AT 11:19:42 ON 06 MAY 2001

L1 STRUCTURE UPLOADED  
L2 50 S L1  
L3 STRUCTURE UPLOADED  
L4 50 S L3  
L5 STRUCTURE UPLOADED  
L6 35 S L5  
L7 428 S L5 FULL

FILE 'CAPLUS, USPATFULL' ENTERED AT 11:23:09 ON 06 MAY 2001

L8 452 S L7  
L9 10 S L8 AND ((CA OR CALCIUM) (P) CHANNEL)  
L10 10 DUP REM L9 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 11:28:55 ON 06 MAY 2001

L11 2 S MIBEFRADIL  
L12 87 S L8 AND ?BIS

FILE 'CAPLUS, USPATFULL' ENTERED AT 11:36:48 ON 06 MAY 2001

L13 98 S L8 AND BIS?  
L14 4 S L8 AND DIMER

FILE 'STNGUIDE' ENTERED AT 11:41:50 ON 06 MAY 2001

FILE 'REGISTRY' ENTERED AT 11:45:18 ON 06 MAY 2001

L15 STRUCTURE UPLOADED  
L16 3 S L15  
L17 31 S L15 FULL

FILE 'CAPLUS, USPATFULL, MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001

L18 11 S L17

FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001

L19 3 S CLENTIAZEM

=> d l18 ti 2-

YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y

L18 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2001 ACS  
TI Synthesis, characterization, and Ca2+ antagonistic activity of diltiazem metabolites

L18 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2001 ACS  
TI Metabolism of diltiazem. I. Structures of new acidic and basic metabolites in rat, dog and man

L18 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2001 ACS  
TI Preparation of 8-chloro-2,3-dihydro-3-hydroxy-2-(4-alkoxyphenyl)-5-[2-(methylamino)ethyl]-1,5-benzothiazepin-4(5H)-ones as cardiovascular agents

L18 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI Benzothiazepine derivatives

L18 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI 2-(4-Benzoyloxyphenyl)-3-acetoxy-5-(2-dimethylaminoethyl)-2,3-dihydro-1,5-benzothiazepin-4-(5H)-ones

L18 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI Benzothiazepine derivatives

L18 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI 3-Acetoxy-2-(p-alkoxyphenyl)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-1,5-benzothiazepin-4(5H)-one derivs.

L18 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI 3-Acetoxy-5-[2-(dimethylamino)ethyl]-2-(p-hydroxyphenyl)-2,3-dihydro-1,5-benzothiazepin-4(5h)-one derivs.

L18 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI 3-Acetoxy-2-[4-(benzyloxy)phenyl]-5-[2-(dimethylamino)ethyl]-2,3-dihydro-1,5-benzothiazepin-4(5H)-one derivs.

L18 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2001 ACS  
 TI Synthesis of the metabolites and related compounds of diltiazem

=> file reg ;s diltiazem

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.31	403.13
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.18

FILE 'REGISTRY' ENTERED AT 11:49:12 ON 06 MAY 2001  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2001 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3  
 DICTIONARY FILE UPDATES: 4 MAY 2001 HIGHEST RN 334719-66-3

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
 for details.

L20 21 DILTIAZEM

=> d

L20 ANSWER 1 OF 21 REGISTRY COPYRIGHT 2001 ACS  
 RN 144604-00-2 REGISTRY  
 CN Butanedioic acid, hydroxy-, (2S)-, compd. with  
 (2S,3S)-3-(acetyloxy)-5-[2-

(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,5-Benzothiazepin-4(5H)-one,  
3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S,3S)-, (2S)-hydroxybutanedioate (1:1) (9CI)

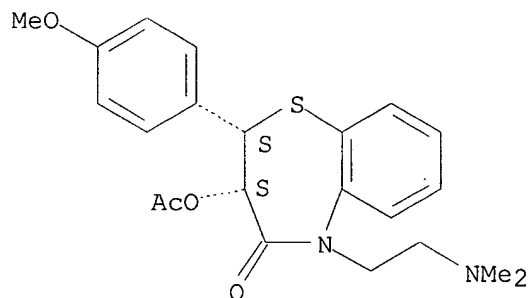
OTHER NAMES:

CN **Diltiazem malate**  
CN MK 793  
FS STEREOSEARCH  
MF C22 H26 N2 O4 S . C4 H6 O5  
CI COM  
SR US Adopted Names Council  
LC STN Files: CA, CAPLUS, DIOGENES, PROMT, TOXLIT, USAN, USPATFULL

CM 1

CRN 42399-41-7  
CMF C22 H26 N2 O4 S

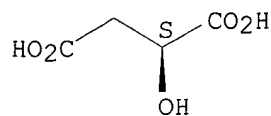
Absolute stereochemistry. Rotation (+).



CM 2

CRN 97-67-6  
CMF C4 H6 O5

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1967 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 11:19:30 ON 06 MAY 2001)

FILE 'REGISTRY' ENTERED AT 11:19:42 ON 06 MAY 2001

L1 STRUCTURE UPLOADED



L2 50 S L1  
L3 STRUCTURE UPLOADED  
L4 50 S L3  
L5 STRUCTURE UPLOADED  
L6 35 S L5  
L7 428 S L5 FULL

FILE 'CAPLUS, USPATFULL' ENTERED AT 11:23:09 ON 06 MAY 2001

L8 452 S L7  
L9 10 S L8 AND ((CA OR CALCIUM) (P) CHANNEL)  
L10 10 DUP REM L9 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 11:28:55 ON 06 MAY 2001

L11 2 S MIBEFRADIL  
L12 87 S L8 AND ?BIS

FILE 'CAPLUS, USPATFULL' ENTERED AT 11:36:48 ON 06 MAY 2001

L13 98 S L8 AND BIS?  
L14 4 S L8 AND DIMER

FILE 'STNGUIDE' ENTERED AT 11:41:50 ON 06 MAY 2001

FILE 'REGISTRY' ENTERED AT 11:45:18 ON 06 MAY 2001

L15 STRUCTURE UPLOADED  
L16 3 S L15  
L17 31 S L15 FULL

FILE 'CAPLUS, USPATFULL, MEDLINE' ENTERED AT 11:46:19 ON 06 MAY 2001

L18 11 S L17

FILE 'REGISTRY' ENTERED AT 11:47:58 ON 06 MAY 2001

L19 3 S CLENTIAZEM

FILE 'CAPLUS' ENTERED AT 11:48:39 ON 06 MAY 2001

FILE 'REGISTRY' ENTERED AT 11:48:42 ON 06 MAY 2001

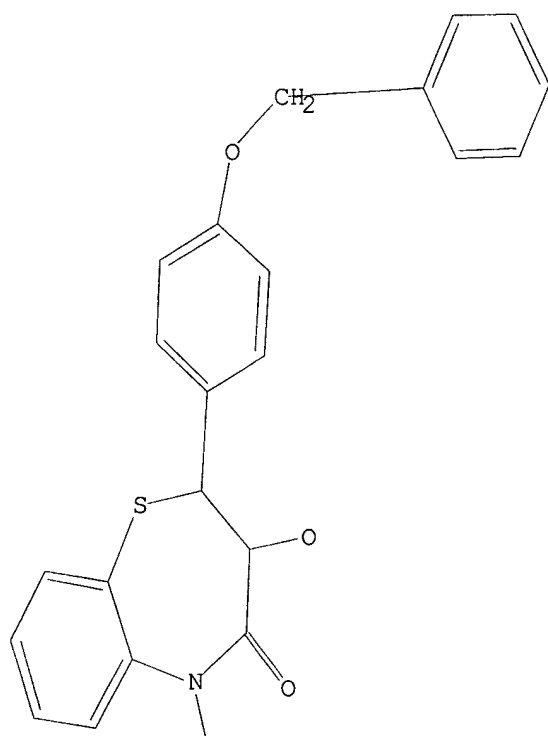
FILE 'REGISTRY' ENTERED AT 11:49:12 ON 06 MAY 2001

L20 21 S DILTIAZEM

=> d l15

L15 HAS NO ANSWERS

L15 STR



Structure attributes must be viewed using STN Express query preparation.

=>

L11 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2001 ACS

RN 116644-53-2 REGISTRY

CN Acetic acid, methoxy-, (1S,2S)-2-[2-[[3-(1H-benzimidazol-2-

yl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-  
2-naphthalenyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Acetic acid, methoxy-, 2-[2-[[3-(1H-benzimidazol-2-

yl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-  
2-naphthalenyl ester, (1S-cis)-

OTHER NAMES:

CN

(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl]methylamino]ethyl]-6-fluoro-  
1-isopropyl-1,2,3,4-tetrahydronaphthalen-2-yl methoxyacetate

CN (1S,2S)-2-[2-[[3-(2-Benzimidazolyl)propyl]methylamino]ethyl]-6-fluoro-  
1,2,3,4-tetrahydro-1-isopropyl-2-naphthyl methoxyacetate

CN **Mibefradil**

FS STEREOSEARCH

MF C29 H38 F N3 O3

CI COM

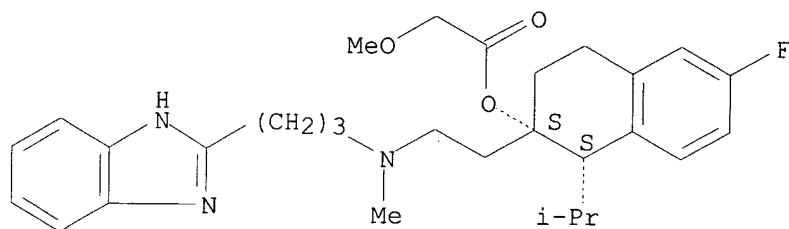
SR CA

LC STN Files: ADISINSIGHT, AIDSLINE, BIOBUSINESS, BIOSIS, CA, CANCERLIT,  
CAPLUS, CASREACT, CIN, DDFU, DIOGENES, DRUGNL, DRUGPAT, DRUGU,  
DRUGUPDATES, IPA, MEDLINE, MRCK\*, PROMT, SYNTHLINE, TOXLINE, TOXLIT,  
USAN, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: WHO

Absolute stereochemistry.



232 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

232 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=>

ACCESSION NUMBER: 1988:549535 CAPLUS  
 DOCUMENT NUMBER: 109:149535  
 TITLE: Preparation of  
 [[(heterocyclylalkyl)amino]ethyl]tetrahy-  
 ydronaphthalenes as cardiovascular agents  
 INVENTOR(S): Branca, Quirico; Jaunin, Roland; Maerki, Hans Peter;  
 Marti, Fraenzi; Ramuz, Henri  
 PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.  
 SOURCE: Eur. Pat. Appl., 37 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 268148	A1	19880525	EP 1987-116251	19871104
EP 268148	B1	19911211		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8705599	A	19880515	DK 1987-5599	19871026
DK 171349	B1	19960916		
CA 1319144	A1	19930615	CA 1987-550190	19871026
CS 264350	B2	19890712	CS 1987-7874	19871103
AT 70267	E	19911215	AT 1987-116251	19871104
ES 2040234	T3	19931016	ES 1987-116251	19871104
ZA 8708362	A	19880727	ZA 1987-8362	19871106
AU 8780909	A1	19880519	AU 1987-80909	19871109
AU 600769	B2	19900823		
IL 84407	A1	19910916	IL 1987-84407	19871109
JP 63139171	A2	19880610	JP 1987-282287	19871110
JP 2504490	B2	19960605		
US 4808605	A	19890228	US 1987-119114	19871110
HU 60251	A2	19920828	HU 1987-5011	19871111
HU 215915	B	19990329		
FI 8705024	A	19880515	FI 1987-5024	19871113
FI 94414	B	19950531		
FI 94414	C	19950911		
NO 8704757	A	19880516	NO 1987-4757	19871113
NO 172237	B	19930315		
NO 172237	C	19930623		
CN 87107875	A	19880525	CN 1987-107875	19871113
CN 1028991	B	19950621		
PRIORITY APPLN. INFO.:			CH 1986-4565	19861114
			EP 1987-116251	19871104

OTHER SOURCE(S): MARPAT 109:149535

IT 116666-64-9P 116666-65-0P 116666-67-2P  
 116666-69-4P 116666-73-0P 116666-76-3P  
 116666-77-4P 116666-78-5P 116666-80-9P  
 116666-93-4P 116667-02-8P 116667-03-9P

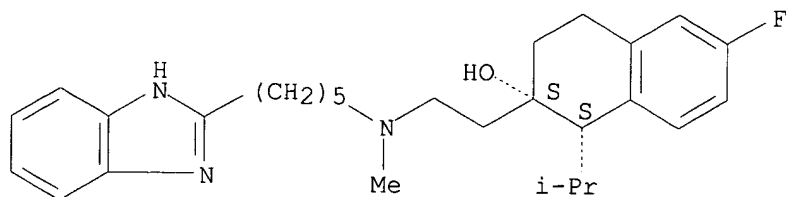
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as cardiovascular agent)

RN 116666-64-9 CAPLUS

CN 2-Naphthalenol,

2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

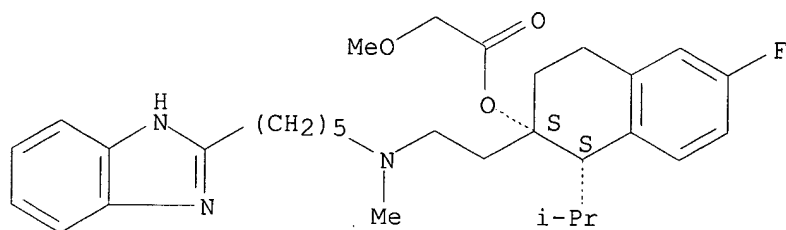


RN 116666-65-0 CAPLUS

CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-

yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-  
2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



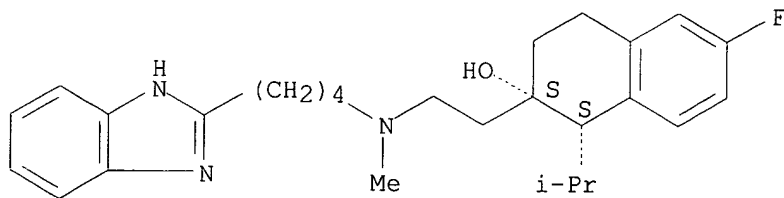
● 2 HCl

RN 116666-67-2 CAPLUS

CN 2-Naphthalenol,

2-[2-[[4-(1H-benzimidazol-2-yl)butyl]methylamino]ethyl]-6-  
fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.

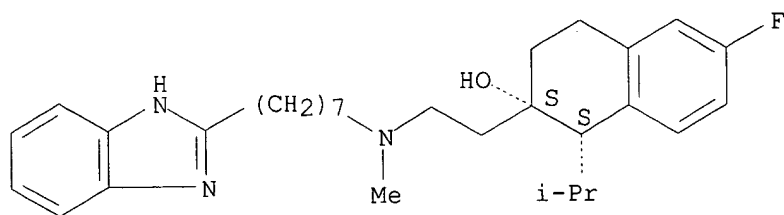


RN 116666-69-4 CAPLUS

CN 2-Naphthalenol,

2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-  
fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, dihydrochloride, (1S-cis)-  
(9CI) (CA INDEX NAME)

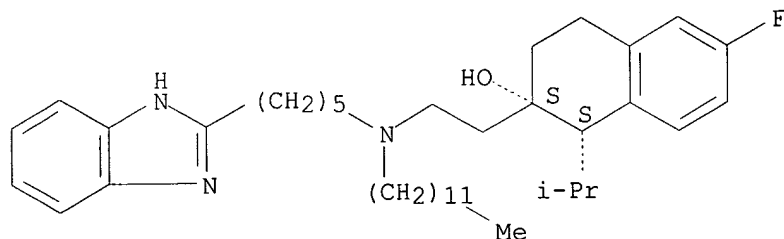
Absolute stereochemistry.



● 2 HCl

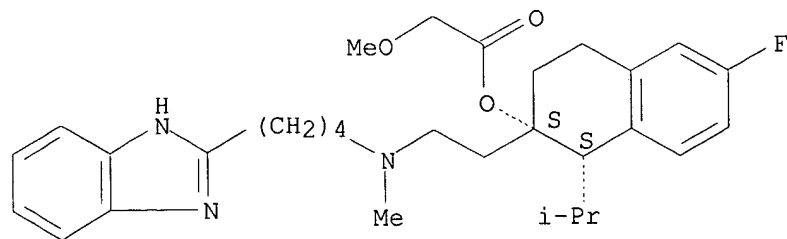
RN 116666-73-0 CAPLUS  
 CN 2-Naphthalenol,  
 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-  
 6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA  
 INDEX  
 NAME)

Absolute stereochemistry.



RN 116666-76-3 CAPLUS  
 CN Acetic acid, methoxy-, 2-[2-[[4-(1H-benzimidazol-2-  
 yl)butyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-  
 2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

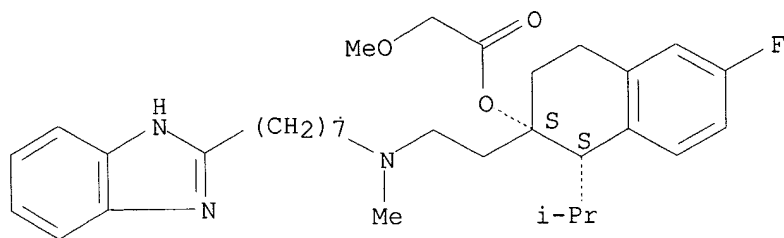


2 HCl

RN 116666-77-4 CAPLUS  
 CN Acetic acid, methoxy-, 2-[2-[[7-(1H-benzimidazol-2-  
 yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-

2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

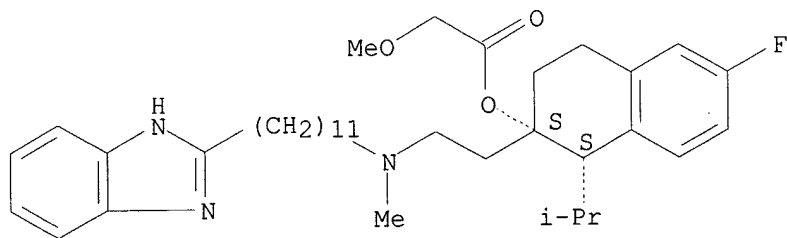


● 2 HCl

RN 116666-78-5 CAPLUS

CN Acetic acid, methoxy-, 2-[2-[[11-(1H-benzimidazol-2-yl)undecyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

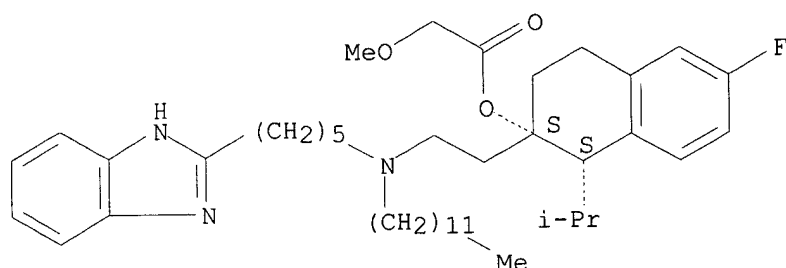


● 2 HCl

RN 116666-80-9 CAPLUS

CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

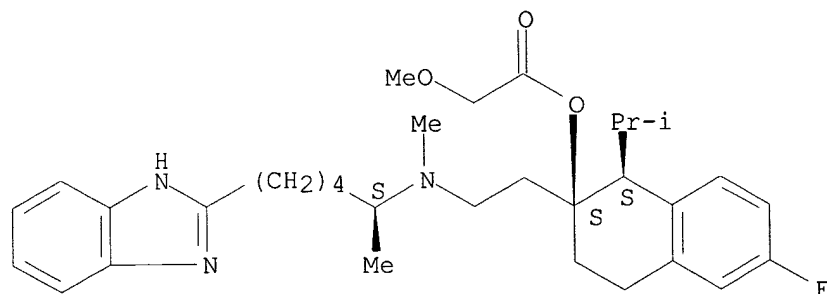


● 2 HCl

RN 116666-93-4 CAPLUS

CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)-1-methylpentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, [1S-[1.alpha.,2.alpha.,2(R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

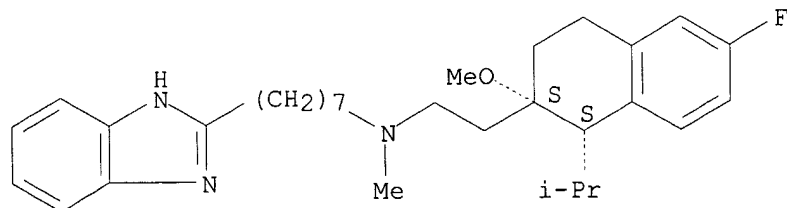


● 2 HCl

RN 116667-02-8 CAPLUS

CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



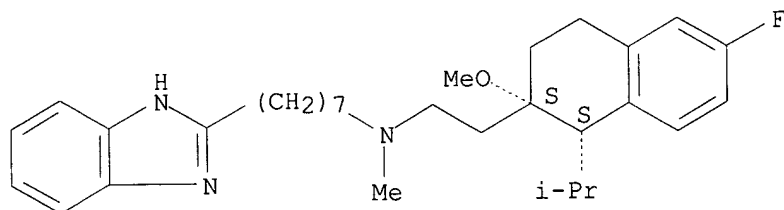
RN 116667-03-9 CAPLUS

CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-



methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-,  
dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

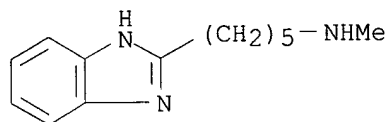
IT 39650-73-2 116666-66-1 116666-68-3  
116666-72-9

RL: RCT (Reactant)

(reaction of, in prepn. of cardiovascular agents)

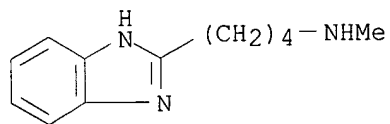
RN 39650-73-2 CAPLUS

CN 1H-Benzimidazole-2-pentanamine, N-methyl- (9CI) (CA INDEX NAME)



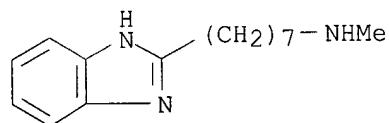
RN 116666-66-1 CAPLUS

CN 1H-Benzimidazole-2-butanamine, N-methyl- (9CI) (CA INDEX NAME)



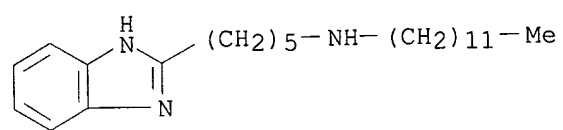
RN 116666-68-3 CAPLUS

CN 1H-Benzimidazole-2-heptanamine, N-methyl- (9CI) (CA INDEX NAME)



RN 116666-72-9 CAPLUS

CN 1H-Benzimidazole-2-pentanamine, N-dodecyl- (9CI) (CA INDEX NAME)



L10 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 2000:405028 CAPLUS

DOCUMENT NUMBER: 133:217516

TITLE: High affinity interaction of mibefradil with voltage-gated **calcium** and sodium **channels**

AUTHOR(S): Eller, Philipp; Berjukov, Stanislav; Wanner, Siegmund;

CORPORATE SOURCE: Huber, Irene; Hering, Steffen; Knaus, Hans-Gunther; Toth, Geza; Kimball, S. David; Striessnig, Jorg  
Institut fur Biochemische Pharmakologie, Innsbruck, A-6020, Austria

SOURCE: Br. J. Pharmacol. (2000), 130(3), 669-677  
CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

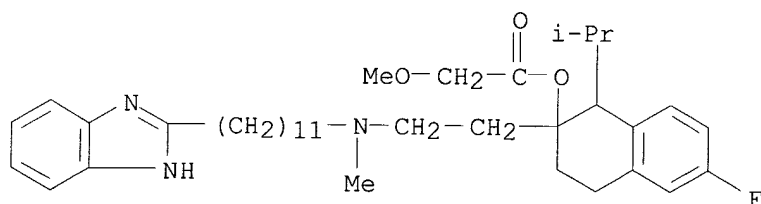
LANGUAGE: English

IT 291307-62-5, Ro 40-6040 291307-63-6, Ro 40-6088

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(high affinity interaction of mibefradil with voltage-gated **calcium** and sodium **channels**)

RN 291307-62-5 CAPLUS

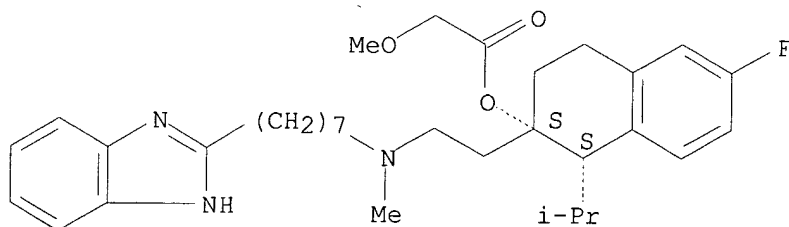
CN Acetic acid, methoxy-, 2-[2-[[11-(1H-benzimidazol-2-yl)undecyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)



RN 291307-63-6 CAPLUS

CN Acetic acid, methoxy-, (1S,2S)-2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46

REFERENCE(S): (1) Aczel, S; Br J Pharmacol 1998, V125, P447 CAPLUS  
(2) Berjukow, S; Br J Pharmacol 1996, V118, P748 CAPLUS  
(3) Bezprozvanny, I; Mol Pharmacol 1995, V48, P540

CAPLUS

- (4) Birnbaumer, L; Neuron 1994, V13, P505 CAPLUS
- (5) Bryson, H; Drugs 1996, V52, P549 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:776400 CAPLUS

DOCUMENT NUMBER: 123:245168

TITLE: Synthesis, Characterization, Spectroscopy, and Magnetism of Dinuclear Azido- and Alkoxy-Bridged Copper(II) Complexes of Bis(2-benzimidazolyl)alkanes. X-ray Structures of

[Cu<sub>2</sub>(tbz)<sub>2</sub>(CH<sub>3</sub>O)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>(CH<sub>3</sub>OH)<sub>2</sub>,  
[Cu<sub>2</sub>(tbz)<sub>2</sub>(NO<sub>3</sub>)(CH<sub>3</sub>O)<sub>2</sub>](NO<sub>3</sub>)(CH<sub>3</sub>OH)<sub>2</sub>, and  
[Cu(tbz)(N<sub>3</sub>)<sub>2</sub>]<sub>2</sub>(CH<sub>3</sub>OH)<sub>2</sub> (tbz = Bis(2-benzimidazolyl)propane)

AUTHOR(S): Van Albada, Gerard A.; Lakin, Miles T.; Veldman, Nora;

CORPORATE SOURCE: Spek, Anthony L.; Reedijk, Jan  
Leiden Institute of Chemistry, Leiden University,  
Leiden, 2300 RA, Neth.

SOURCE: Inorg. Chem. (1995), 34(19), 4910-17  
CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A group of new compds. Cu(L)(sol-)(A-)(Hsol), where A = ClO<sub>4</sub>-, CF<sub>3</sub>SO<sub>3</sub>-, BF<sub>4</sub>-, and NO<sub>3</sub>-, L = bis(2-benzimidazolyl)propane (abbreviated as tbz) and bis(2-benzimidazolyl)butane (abbreviated as qbz), and Hsol = MeOH and EtOH, and [Cu(tbz)(N<sub>3</sub>)(Hsol)] was prepd. and characterized structurally, magnetically, and spectroscopically. Three representative compds. [Cu<sub>2</sub>(tbz)<sub>2</sub>(MeO)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>(MeOH)<sub>2</sub> (1), [Cu<sub>2</sub>(tbz)<sub>2</sub>(NO<sub>3</sub>)(MeO)<sub>2</sub>](NO<sub>3</sub>)(MeOH)<sub>2</sub> (5), and [Cu(tbz)(N<sub>3</sub>)<sub>2</sub>]<sub>2</sub>(MeOH)<sub>2</sub> (13) were characterized structurally with x-ray diffraction. Crystal data for 1: monoclinic, space group P2<sub>1</sub>/c

with

a 9.6863(10), b 12.9445(10), c 19.394(2) .ANG., .beta.  
113.259(10).degree., and Z = 2. Crystal data for 5: monoclinic, space group P2<sub>1</sub> with a 9.5497(6), b 12.5073(7), c 17.5920(12) .ANG., .beta.  
90.996(6).degree., and Z = 2. Crystal data for 13: orthorhombic, space group Pbca with a 11.3325(7), b 18.7096(16), c 19.2011(16) .ANG., and Z = 4. The structure refinement converged to wR<sub>2</sub> = 0.1381, R<sub>1</sub> = 0.0534 for

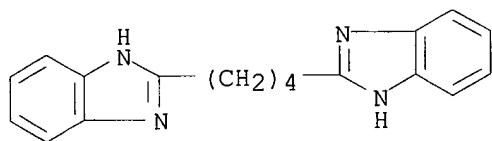
1,

wR<sub>2</sub> = 0.0674, R<sub>1</sub> = 0.0271 for 5, and wR<sub>2</sub> = 0.1119, R<sub>1</sub> = 0.0701 for 13. The structures 1 and 5 consist of dinuclear units with bridging methoxo groups and one ligand linked to each Cu via the N, providing square

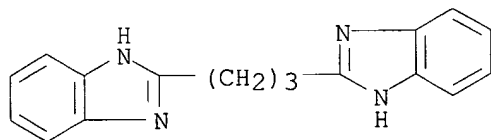
planar

CuN<sub>2</sub>O<sub>2</sub> chromophores. Structure 5 consists of a dinuclear unit in which one of the Cu atoms is linked to a nitrate O, to yield a unit with two different Cu environments, one square planar and the other square pyramidal. Structure 13 consists also of dinuclear units with the two Cu atoms bridged by .mu.-(1,1)-azido groups. Also each Cu is surrounded by two nitrogens of the ligand and a N of a nonbridging end-on .mu.-(1,1)-azido moiety resulting in a distorted square pyramidal geometry. The Cu-Cu distances (.ANG.) within the dinuclear units are as follows: 1, 2.9827(6); 5, 3.0072(4); 13, 3.2422(9). The Cu-O-Cu bridging angles (deg) are as follows: 1, 102.89(14); 5, 103.97(9), 103.06(9).degree.. The Cu-N-Cu bridging angle for 13 is 104.66(17).degree.. Far-IR spectroscopy shows bands which are characteristic for the bridging Cu<sub>2</sub>O<sub>2</sub>N<sub>4</sub> chromophore; Cu-O vibrations are found at .apprx.457 and 330 cm<sup>-1</sup> for the ethoxo-bridged compds. and at .apprx.390 and 232 cm<sup>-1</sup> for the methoxo-bridged compds. The magnetic susceptibility measurements of the alkoxy-bridged compds. display a diamagnetic behavior below room temp. with an estd. exchange parameter 2J of <-600 cm<sup>-1</sup>. These dinuclear species are EPR silent, and only a weak signal of monomeric impurities is obsd. The .mu.-(1,1)-azido-bridged dimer shows a ferromagnetic behavior with a calcd. J value of +23

cm-1 and a weak, very broad isotropic EPR signal at  $g = 2.14$ .  
 IT **4746-56-9**, 1,4-Bis(2-benzimidazolyl)butane  
 RL: RCT (Reactant)  
 (for prepn. of copper dinuclear alkoxo-bridged complexes)  
 RN 4746-56-9 CAPLUS  
 CN 1H-Benzimidazole, 2,2'-(1,4-butanediyl)bis- (9CI) (CA INDEX NAME)



IT **7147-66-2**, 1,3-Bis(2-benzimidazolyl)propane  
 RL: RCT (Reactant)  
 (for prepn. of copper dinuclear azido-, alkoxo- and  
 alkoxo/nitrato-bridged complexes)  
 RN 7147-66-2 CAPLUS  
 CN 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis- (9CI) (CA INDEX NAME)



=>

L11 ANSWER 2 OF 2 USPATFULL

ACCESSION NUMBER: 89:15067 USPATFULL

TITLE: Tetrahydronaphthalene derivatives as calcium antagonists

INVENTOR(S): Branca, Quirico, Basel, Switzerland  
Jaunin, Roland, Basel, Switzerland  
Maki, Hans P., Basel, Switzerland  
Marti, Franzi, Riehen, Switzerland  
Ramuz, Henri, Birsfelden, Switzerland  
PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., Nutley, NJ, United States  
(U.S. corporation)

	NUMBER	DATE
PATENT INFORMATION:	US 4808605	19890228
APPLICATION INFO.:	US 1987-119114	19871110 (7)

	NUMBER	DATE
PRIORITY INFORMATION:	CH 1986-4565	19861114
DOCUMENT TYPE:	Utility	
PRIMARY EXAMINER:	Schwartz, Richard A.	
LEGAL REPRESENTATIVE:	Saxe, Jon S.; Leon, Bernard S.; Boxer, Matthew	
NUMBER OF CLAIMS:	21	
EXEMPLARY CLAIM:	19	
LINE COUNT:	2166	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 116666-64-9P 116666-65-0P 116666-67-2P  
116666-69-4P 116666-73-0P 116666-76-3P  
116666-77-4P 116666-78-5P 116666-80-9P  
116666-93-4P 116667-02-8P 116667-03-9P  
(prepn. of, as cardiovascular agent)

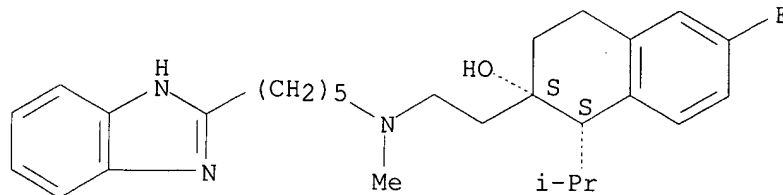
RN 116666-64-9 USPATFULL

CN 2-Naphthalenol,

2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA

INDEX  
NAME)

Absolute stereochemistry.

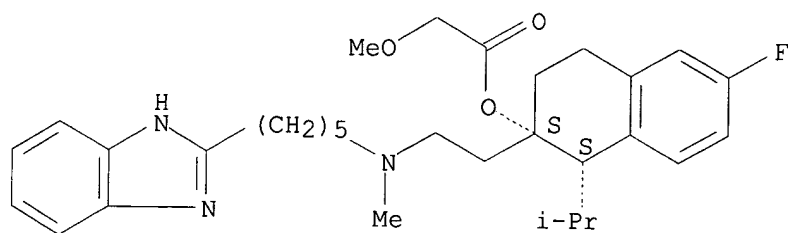


RN 116666-65-0 USPATFULL

CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

RN 116666-67-2 USPATFULL

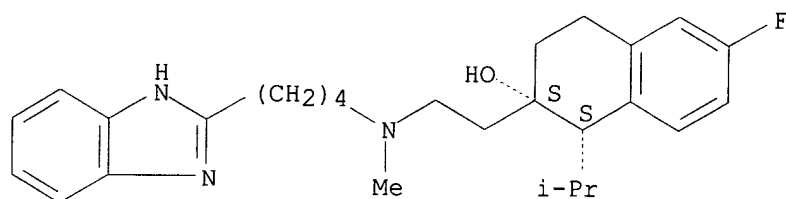
CN 2-Naphthalenol,

2-[2-[[4-(1H-benzimidazol-2-yl)butyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA

INDEX

NAME)

Absolute stereochemistry.



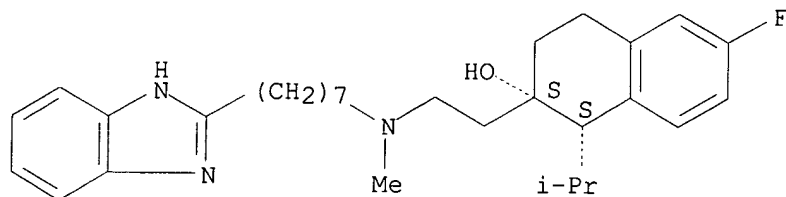
RN 116666-69-4 USPATFULL

CN 2-Naphthalenol,

2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, dihydrochloride, (1S-cis)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

RN 116666-73-0 USPATFULL

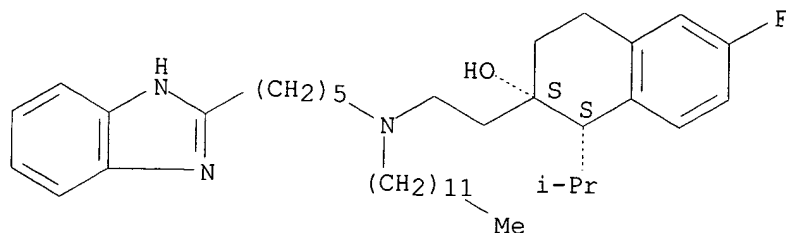
CN 2-Naphthalenol,

2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-



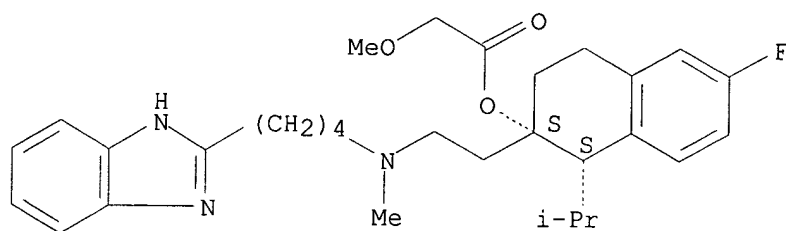
6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-, (1S-cis)- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



RN 116666-76-3 USPATFULL  
CN Acetic acid, methoxy-, 2-[2-[[4-(1H-benzimidazol-2-yl)butyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI)  
(CA INDEX NAME)

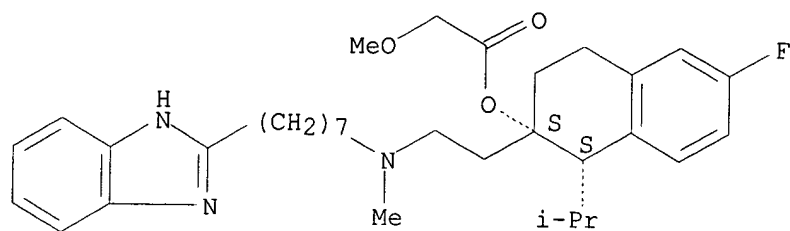
Absolute stereochemistry.



● 2 HCl

RN 116666-77-4 USPATFULL  
CN Acetic acid, methoxy-, 2-[2-[[7-(1H-benzimidazol-2-yl)heptyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



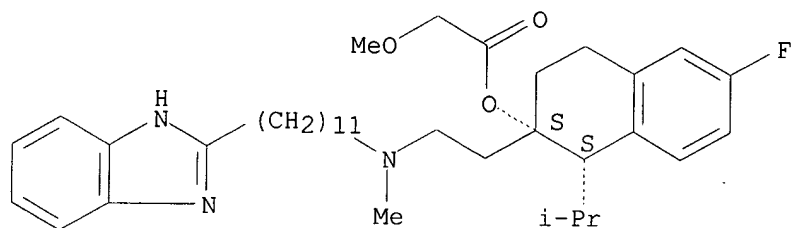
● 2 HCl

RN 116666-78-5 USPATFULL

CN Acetic acid, methoxy-, 2-[2-[[11-(1H-benzimidazol-2-yl)undecyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



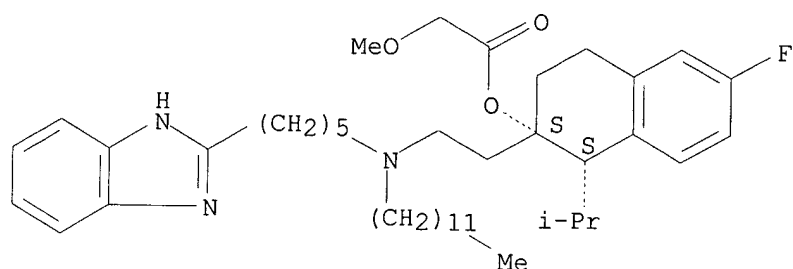
● 2 HCl

RN 116666-80-9 USPATFULL

CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)pentyl]dodecylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, (1S-cis)- (9CI)

(CA INDEX NAME)

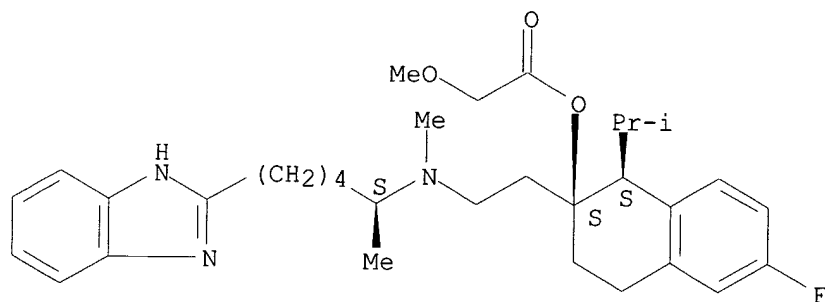
Absolute stereochemistry.



● 2 HCl

RN 116666-93-4 USPATFULL  
 CN Acetic acid, methoxy-, 2-[2-[[5-(1H-benzimidazol-2-yl)-1-methylpentyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl ester, dihydrochloride, [1S-[1.alpha.,2.alpha.,2(R\*)]]- (9CI) (CA INDEX NAME)

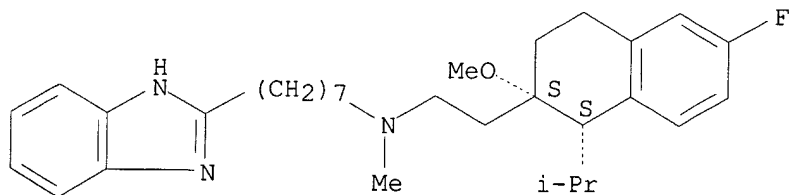
Absolute stereochemistry.



● 2 HCl

RN 116667-02-8 USPATFULL  
 CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-, (1S-cis)- (9CI) (CA INDEX NAME)

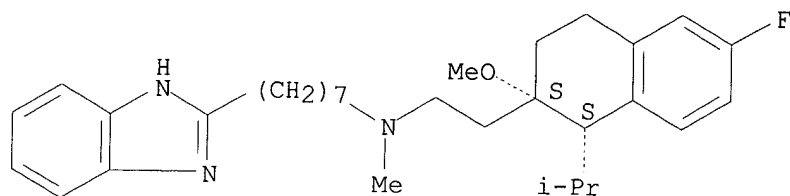
Absolute stereochemistry.



RN 116667-03-9 USPATFULL  
 CN 1H-Benzimidazole-2-heptanamine, N-[2-[6-fluoro-1,2,3,4-tetrahydro-2-methoxy-1-(1-methylethyl)-2-naphthalenyl]ethyl]-N-methyl-,

dihydrochloride, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



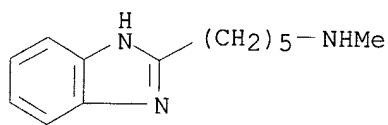
● 2 HCl

IT 39650-73-2 116666-66-1 116666-68-3  
116666-72-9

(reaction of, in prepn. of cardiovascular agents)

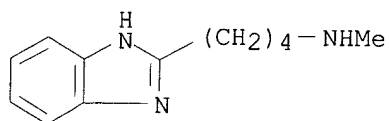
RN 39650-73-2 USPATFULL

CN 1H-Benzimidazole-2-pentanamine, N-methyl- (9CI) (CA INDEX NAME)



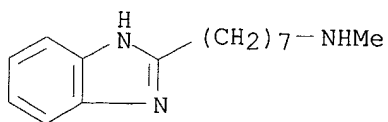
RN 116666-66-1 USPATFULL

CN 1H-Benzimidazole-2-butanamine, N-methyl- (9CI) (CA INDEX NAME)



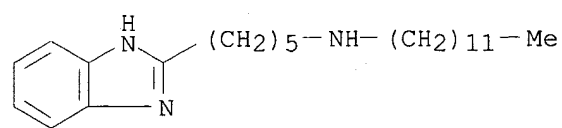
RN 116666-68-3 USPATFULL

CN 1H-Benzimidazole-2-heptanamine, N-methyl- (9CI) (CA INDEX NAME)



RN 116666-72-9 USPATFULL

CN 1H-Benzimidazole-2-pentanamine, N-dodecyl- (9CI) (CA INDEX NAME)



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Attachment to  
EP 0122488

RN 94637-59-9 REGISTRY

CN Piperazine, 1,1'-(1,3-propanediyl)bis[4-[bis(4-chlorophenyl)methyl]-,  
dihydrochloride (9CI) (CA INDEX  
NAME)

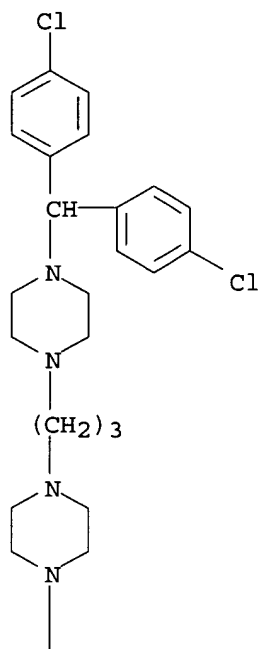
MF C37 H40 Cl4 N4 . 2 Cl H

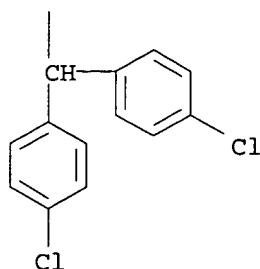
LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	4
C4N2	NC2NC2	6	C4N2	46.383.1	2

PAGE 1-A





● 2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

## REFERENCE 1

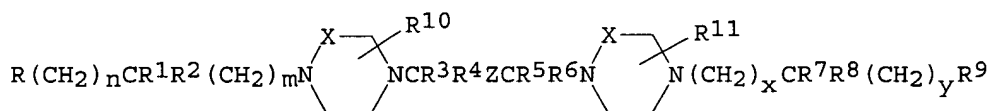
AN 102:78912 CA  
 TI Bis(piperazinyl- or -homopiperazinyl)alkanes  
 IN Devlin, John P.; McNeil, Daniel W.; Keirns, James J.; Barsumian, Edward  
 L.  
 PA Boehringer Ingelheim Ltd., USA  
 SO Eur. Pat. Appl., 53 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA German  
 IC C07D403-06; A61K031-495  
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63

## FAN.CNT 2

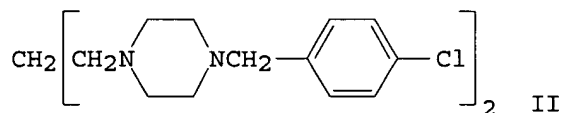
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 122488	A1	19841024	EP 1984-102979	19840317
	EP 122488	B1	19890607		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	AT 43843	E	19890615	AT 1984-102979	19840317
	FI 8401081	A	19840922	FI 1984-1081	19840319
	FI 80269	B	19900131		
	FI 80269	C	19900510		
	DK 8401601	A	19840922	DK 1984-1601	19840320
	DK 166022	B	19930301		
	DK 166022	C	19930802		
	NO 8401078	A	19840924	NO 1984-1078	19840320
	NO 162907	B	19891127		
	NO 162907	C	19900307		
	AU 8425891	A1	19840927	AU 1984-25891	19840320
	AU 568122	B2	19871217		
	HU 34016	O	19850128	HU 1984-1102	19840320
	HU 191599	B	19870330		
	DD 219642	A5	19850313	DD 1984-261058	19840320
	ES 530762	A1	19850616	ES 1984-530762	19840320
	ZA 8402037	A	19851224	ZA 1984-2037	19840320
	CA 1218652	A1	19870303	CA 1984-450025	19840320
	PL 141127	B1	19870630	PL 1984-246774	19840320

IL 71291	A1	19871130	IL 1984-71291	19840320
CS 254971	B2	19880215	CS 1984-1960	19840320
JP 59176265	A2	19841005	JP 1984-54152	19840321
ES 535438	A1	19850916	ES 1984-535438	19840827
ES 535439	A1	19850916	ES 1984-535439	19840827
ES 535440	A1	19850916	ES 1984-535440	19840827
SU 1568887	A3	19900530	SU 1986-4027076	19860312
SU 1574174	A3	19900623	SU 1986-4027087	19860312
CS 254998	B2	19880215	CS 1986-5529	19860721
PRAI US 1983-477008		19830321		
EP 1984-102979		19840317		
CS 1984-1960		19840320		

GI



I



AB The title compds. [I; R, R<sub>9</sub> = (un)substituted Ph; R<sub>1</sub>, R<sub>8</sub> = H, alkoxy carbonyl, Me, HOCH<sub>2</sub>, CO<sub>2</sub>H, OH, Ph, 4-ClC<sub>6</sub>H<sub>4</sub>; R<sub>2</sub>-R<sub>7</sub> = H, Me; R<sub>10</sub>, R<sub>11</sub> = 0-4 Me groups; R<sub>1</sub>R<sub>2</sub>, R<sub>3</sub>R<sub>4</sub>, R<sub>5</sub>R<sub>6</sub>, R<sub>7</sub>R<sub>8</sub> = O; X = CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>; Z = Cl-2 alkylene, hydroxyalkylene; n, m, x, y = 0-3; n + m, x + y .ltoreq. 4] were prepd. Thus, 1-[(4-chlorophenyl)methyl]piperazine was refluxed 17 h in EtOH with Br(CH<sub>2</sub>)<sub>3</sub>Cl and the product in Et<sub>2</sub>O treated with gaseous HCl to give 39% II.4HCl (III). III inhibited mediator release from a rat mast cell prepn. with an IC<sub>50</sub> of 3 .mu.M.

ST alkylenebispiperazine prepn anti allergy anti inflammatory; piperazine alkylenebis; alkylation piperazine homopiperazine

IT Inflammation inhibitors and Antiarthritics (alkylenebis[piperazine] derivs.)

IT Allergy (inhibitors, alkylenebis[piperazine] derivs.)

IT Alkylation (of piperazines and homopiperazines)

IT 23145-88-2 40389-65-9  
RL: RCT (Reactant); RACT (Reactant or reagent) (acylation and alkylation of)

IT 1663-67-8 15486-96-1  
RL: RCT (Reactant); RACT (Reactant or reagent) (acylation of (chlorobenzyl)piperazine)

IT 64473-34-3 90876-16-7  
RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation by, of piperazines)

IT 106-55-8 2759-28-6 5321-49-3 17532-19-3 21867-69-6 23145-91-7  
23173-57-1 27469-61-0



39577-03-2    41298-98-0    55455-93-1    55513-17-2    69628-75-7  
 91345-62-9    94637-81-7    94637-82-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (alkylation of)  
 IT    107-80-2    109-70-6    110-52-1    22286-82-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (alkylation of piperazines by)  
 IT    110-85-0, reactions    19479-82-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzylation of)  
 IT    352-11-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzylation of piperazine by)  
 IT    75462-56-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (benzylation with, of trimethylene bis[piperazine])  
 IT    59214-26-5P    70931-28-1P    94637-78-2P    94637-79-3P    94637-80-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and alkylation of)  
 IT    94637-89-5P    94637-90-8P    94637-91-9P    94637-95-3P    94637-96-4P  
 94637-97-5P    94637-99-7P  
 94638-00-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and antiallergy-antiinflammatory activity of)  
 IT    94637-93-1P    94637-94-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and borohydride redn. of)  
 IT    94637-98-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and ether cleavage of)  
 IT    94637-92-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and sapon. of)  
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 94637-36-2P    94637-37-3P  
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 94637-43-1P    94637-44-2P  
       94637-45-3P    94637-46-4P    94637-47-5P    94637-48-6P    94637-49-7P  
 94637-50-0P    94637-51-1P  
       94637-52-2P    94637-53-3P    94637-54-4P    94637-55-5P    94637-56-6P  
 94637-57-7P    94637-58-8P  
       94637-59-9P    94637-60-2P    94637-61-3P    94637-62-4P    94637-63-5P  
 94637-64-6P    94637-65-7P  
       94637-66-8P    94637-67-9P    94637-68-0P    94637-69-1P    94637-70-4P  
 94637-71-5P    94637-72-6P  
       94637-73-7P    94637-74-8P    94637-75-9P    94637-76-0P    94644-67-4P  
 94655-69-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, as antiallergy-antiinflammatory agent)  
 IT    94637-77-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn., acetylation, and butylation of)